Geometric uncertainty relation for mixed quantum states

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The phase space of a unitarily evolving quantum system in a mixed state consists of isospectral density operators. In this paper we equip the spaces of isospectral density operators with natural Riemannian and symplectic structures, and we derive a geometric uncertainty relation for observables acting on systems in mixed states. Moreover, we give a geometric proof of the Robertson-Schrödinger uncertainty relation, and we compare the two uncertainty relations.

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I. INTRODUCTION

Classical mechanics is basically a geometric theory, while the traditional mathematical formulation of quantum mechanics is functional analytic. Geometric quantum mechanics seeks to unify these seemingly different approaches to mechanics.

Classical and quantum mechanical systems have in common that their phase spaces are symplectic manifolds, and that their observables give rise to symplectic flows [1–4]. But quantum systems exhibit characteristics that have no classical counterparts. One is the impossibility to fully predict results of measurements.

In classical mechanics, observables are represented by real-valued functions, and the result of a measurement of an observable equals the value of the corresponding function at the point in phase space that labels the system's state. This means that in classical mechanics, the results of measurements are completely predictable. The situation in quantum mechanics, however, is quite different. There, observables are represented by self-adjoint operators, and due to intrinsic properties of quantum systems, only expectation values and uncertainties of observables can be calculated; the actual value of an observable can, in general, not be known prior to measurement. Furthermore, there is a limit to the precision with which values of pairs of observables can be known simultaneously. This is the famous quantum uncertainty principle.

A quantum system prepared in a pure state can be modeled on a projective Hilbert space equipped with a distinguished Kähler metric, called the Fubini-Study Kähler metric. The real and imaginary parts of this metric (suitably scaled) provide the projective Hilbert space with Riemannian and symplectic structures, respectively, and hence with Riemann and Poisson brackets. It has been shown, see, e.g., [3], that for observables acting on a system in a pure state, the Robertson-Schrödinger uncertainty principle [5, 6] can be expressed entirely in terms of the Riemann and Poisson brackets of the observables expectation value functions.

The state of an experimentally prepared quantum system usually exhibits classical uncertainty; the state is mixed, i.e., is in an incoherent superposition of pure states. Mixed states are commonly represented by density operators, and thus the phase spaces of quantum systems in mixed states are made up of such.

If a quantum system evolves according to a von Neumann equation, then the spectrum of the density operator representing the system's prepared state will be preserved. In this paper we equip the spaces isospectral density operators with Riemannian and symplectic structures, and we derive a geometric uncertainty relation for observables acting on systems in mixed states. We also give a geometric proof of the Robertson-Schrödinger uncertainty relation, and we compare the strengths of two uncertainty relations.

A. Notation

Operators on Hermitian space $\mathbb{C}^k$ will be represented by matrices with respect to the canonical basis, whose j^{th} member we denote by e_j. In particular, we write $\mathbf{1}_k$ and $\mathbf{0}_k$ for the matrices representing the identity and zero operator, respectively.

We will primarily be interested in finitely mixed quantum systems that evolve unitarily. They will be modeled on a Hilbert space $\mathscr{H}$, and their states will be represented by density operators of finite rank. Recall that a density operator is a Hermitian, nonnegative operator with unit trace. We write $\mathscr{D}(\mathscr{H})$ for the space of density operators on $\mathscr{H}$.

An elementary but, in this context, crucial fact is that a density operator ρ on $\mathscr{H}$ of rank at most k can be factorized as $\rho = \psi\psi^\dagger$ for some linear map $\psi : \mathbb{C}^k \to \mathscr{H}$ of unit norm. We write Ł$(\mathbb{C}^k, \mathscr{H})$ for the space of linear maps from $\mathbb{C}^k$ to $\mathscr{H}$ equipped with the Hilbert-Schmidt Hermitian product, and G and Ω for $2\hbar$ times the real and imaginary parts, respectively, of this product:

$$G(X,Y) = \hbar\,\mathrm{Tr}(X^\dagger Y + Y^\dagger X), \tag{1}$$

$$\Omega(X,Y) = -i\hbar\,\mathrm{Tr}(X^\dagger Y - Y^\dagger X). \tag{2}$$

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II. GEOMETRIC STRUCTURES ON ORBITS OF ISOSPECTRAL DENSITY OPERATORS

A density operator whose evolution is governed by a von Neumann equation remains in a single orbit of the left conjugation action of the unitary group of $\mathscr{H}$ on $\mathscr{D}(\mathscr{H})$. The orbits of this action are in one-to-one correspondence with the possible spectra for density operators on $\mathscr{H}$, where by the *spectrum* of a density operator of rank k we mean the decreasing sequence $\sigma = (p_1, p_2, \dots, p_k)$ of its, not necessarily distinct, positive eigenvalues. Throughout this paper we fix σ, and write $\mathscr{D}(\sigma)$ for the corresponding orbit.

Let $\mathscr{S}(\sigma) = \{\psi \in \text{Ł}(\mathbb{C}^k, \mathscr{H}) : \psi^\dagger\psi = P(\sigma)\}$, where $P(\sigma)$ is the diagonal $k \times k$ matrix that has σ as its diagonal, and define

$$\pi : \mathscr{S}(\sigma) \to \mathscr{D}(\sigma), \quad \psi \mapsto \psi\psi^\dagger. \tag{3}$$

Then π is a principal fiber bundle with right acting gauge group $\mathscr{U}(\sigma) = \{U \in \mathscr{U}(k) : UP(\sigma) = P(\sigma)U\}$, whose Lie algebra is $\mathfrak{u}(\sigma) = \{\xi \in \mathfrak{u}(k) : \xi P(\sigma) = P(\sigma)\xi\}$. Observe that if the elements in $\mathscr{D}(\sigma)$ represent pure states, i.e., if $\sigma = (1)$, then $\mathscr{D}(\sigma)$ is the projective space over $\mathscr{H}$, and (3) is the (generalized) Hopf bundle.

A. Riemannian and symplectic structures

A gauge invariant Riemannian metric on $\mathscr{S}(\sigma)$ is given by the restriction of G in (1) to $\mathscr{S}(\sigma)$. We define the *vertical* and *horizontal bundles* over $\mathscr{S}(\sigma)$ to be the subbundles $\mathrm{V}\mathscr{S}(\sigma) = \operatorname{Ker}\pi_*$ and $\mathrm{H}\mathscr{S}(\sigma) = \mathrm{V}\mathscr{S}(\sigma)^\perp$ of the tangent bundle $\mathrm{T}\mathscr{S}(\sigma)$. Here π_* is the differential of π and $^\perp$ denotes orthogonal complement with respect to G. Vectors in $\mathrm{V}\mathscr{S}(\sigma)$ and $\mathrm{H}\mathscr{S}(\sigma)$ are called vertical and horizontal, respectively, and we equip $\mathscr{D}(\sigma)$ with the unique metric g that makes π a Riemannian submersion. Thus, g is such that the restriction of π_* to each fiber of $\mathrm{H}\mathscr{S}(\sigma)$ is an isometry.

The infinitesimal generators of the gauge group action yield canonical isomorphisms between $\mathfrak{u}(\sigma)$ and the fibers in $\mathrm{V}\mathscr{S}(\sigma)$:

$$\mathfrak{u}(\sigma) \ni \xi \mapsto \psi\xi \in \mathrm{V}_\psi\mathscr{S}(\sigma).$$

Furthermore, $\mathrm{H}\mathscr{S}(\sigma)$ is the kernel bundle of the gauge invariant *mechanical connection form* $\mathscr{A} : \mathrm{T}\mathscr{S}(\sigma) \to \mathfrak{u}(\sigma)$ defined by $\mathscr{A}_\psi = I_\psi^{-1} J_\psi$, where $I : \mathscr{S}(\sigma) \times \mathfrak{u}(\sigma) \to \mathfrak{u}(\sigma)^*$ and $J : \mathrm{T}\mathscr{S}(\sigma) \to \mathfrak{u}(\sigma)^*$ are the *locked inertia tensor* and *momentum map*, respectively:

$$I_\psi\xi \cdot \eta = G(\psi\xi, \psi\eta), \quad J_\psi(X) \cdot \eta = G(X, \psi\eta).$$

The inertia tensor is of *constant bi-invariant type* since it is an adjoint-invariant form on $\mathfrak{u}(\sigma)$ which is independent of ψ in $\mathscr{S}(\sigma)$. Hence, it defines a metric $\xi \cdot \eta$ on $\mathfrak{u}(\sigma)$. Explicitly,

$$\xi \cdot \eta = \hbar \operatorname{Tr}\Big(\big(\xi^\dagger\eta + \eta^\dagger\xi\big)P(\sigma)\Big). \tag{4}$$

Using (4) we can derive an explicit formula for the connection form. Indeed, if $m_1, m_2, \dots, m_l$ are the multiplicities of the different eigenvalues in σ, with m_1 being the multiplicity of the greatest eigenvalue, m_2 the multiplicity of the second greatest eigenvalue, etc., and if for $j = 1, 2, \dots, l$,

$$E_j = \operatorname{diag}(\mathbf{0}_{m_1}, \dots, \mathbf{0}_{m_{j-1}}, \mathbf{1}_{m_j}, \mathbf{0}_{m_{j+1}}, \dots, \mathbf{0}_{m_l}),$$

then a straightforward application of (4) yields

$$\sum_j E_j\psi^\dagger X E_j P(\sigma)^{-1} \cdot \eta = J_\psi(X) \cdot \eta, \quad X \in \mathrm{T}_\psi\mathscr{S}(\sigma).$$

We conclude that

$$\mathscr{A}_\psi(X) = \sum_j E_j\psi^\dagger X E_j P(\sigma)^{-1}. \tag{5}$$

The form Ω in (2) is a symplectic form on $\text{Ł}(\mathbb{C}^k, \mathscr{H})$. Montgomery [7] showed that the bundles (3) are the reduced space submersions obtained by symplectic reduction by the right action of $\mathscr{U}(k)$ on $\text{Ł}(\mathbb{C}^k, \mathscr{H})$. Since the action is symplectic, it follows from a celebrated result by Marsden and Weinstein [8, Th 1] that there is a unique symplectic structure ω on $\mathscr{D}(\sigma)$ such that $\pi^*\omega$ equals the restriction of Ω to $\mathscr{S}(\sigma)$.

For each observable $\hat{A}$ on $\mathscr{H}$, define the *expectation value function* A and associated *Hamiltonian vector field* X_A on $\mathscr{D}(\sigma)$ by

$$A(\rho) = \operatorname{Tr}(\hat{A}\rho), \quad dA = \iota_{X_A}\omega.$$

Also, let $X_{\hat{A}}$ be the gauge invariant vector field on $\mathscr{S}(\sigma)$ defined by

$$X_{\hat{A}}(\psi) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left[\exp\Big(\frac{\varepsilon}{i\hbar}\hat{A}\Big)\psi\right]_{\varepsilon=0}. \tag{6}$$

Then $\iota_{\pi_*(X_{\hat{A}})}\omega = dA$, which means that $X_{\hat{A}}$ projects onto X_A.

An observable $\hat{A}$ is *parallel* at a density operator ρ if $X_{\hat{A}}$ is horizontal at some, hence every, element in the fiber over ρ. We will show that the uncertainty of a parallel observable is proportional to the norm of the Hamiltonian vector field associated with the observable's expectation value function.

The locked inertia tensor provides a means to measure deviation from parallelism: Given an observable $\hat{A}$ we define a $\mathfrak{u}(\sigma)$-valued field ξ_A on $\mathscr{D}(\sigma)$ by $\pi^*\xi_A = \mathscr{A} \circ X_{\hat{A}}$. Then $\xi_A \cdot \xi_A$ equals the square of the norm of the vertical part of $X_{\hat{A}}$. It is an interesting fact that ξ_A contains complete information about the expectation values of $\hat{A}$, see (8) below.

III. GEOMETRIC UNCERTAINTY ESTIMATES

The precision to which the value of an observable $\hat{A}$ can be known is quantified by its *uncertainty*,

$$\Delta A(\rho) = \sqrt{\operatorname{Tr}(\hat{A}^2\rho) - \operatorname{Tr}(\hat{A}\rho)^2},$$

and the precision to which the values of two observables $\hat{A}$ and $\hat{B}$ can be known simultaneously is limited by the *Robertson-Schrödinger uncertainty relation* [5, 6]:

$$\Delta A \Delta B \geq \sqrt{((A,B) - AB)^2 + [A,B]^2}. \tag{7}$$

Here (A,B) and $[A,B]$ are the expectation value functions of the symmetric and antisymmetric products of $\hat{A}$ and $\hat{B}$:

$$(\hat{A},\hat{B}) = \frac{1}{2}(\hat{A}\hat{B}+\hat{B}\hat{A}), \quad [\hat{A},\hat{B}] = \frac{1}{2i}(\hat{A}\hat{B}-\hat{B}\hat{A}).$$

In this section we derive a lower bound for $\Delta A\Delta B$ that involves only the Riemannian and symplectic products of the Hamiltonian vector fields of A and B. Thus, we derive a geometric uncertainty relation for observables of quantum systems in mixed states. Also, we compare it with (7).

A. A geometric uncertainty relation

Let $\hat{A}$ and $\hat{B}$ be two observables, and χ be the unit vector $\mathbf{1}_k/i\sqrt{2\hbar}$ in $\mathfrak{u}(\sigma)$. The expectation value functions of $\hat{A}$ and $\hat{B}$ are proportional to the lengths of the projections of ξ_A and ξ_B, respectively, on χ:

$$A = \sqrt{\frac{\hbar}{2}}\chi\cdot\xi_A, \quad B = \sqrt{\frac{\hbar}{2}}\chi\cdot\xi_B. \tag{8}$$

Furthermore,

$$(A,B) = \frac{\hbar}{2}\left(\{A,B\}_g + \xi_A\cdot\xi_B\right), \quad [A,B] = \frac{\hbar}{2}\{A,B\}_\omega, \tag{9}$$

where $\{A,B\}_g = g(X_A,X_B)$ and $\{A,B\}_\omega = \omega(X_A,X_B)$ are the *Riemann* and *Poisson brackets* of A and B. Consequently,

$$(A,B) - AB = \frac{\hbar}{2}\left(\{A,B\}_g + \xi_A^\perp\cdot\xi_B^\perp\right), \tag{10}$$

where $\xi_A^\perp$ and $\xi_B^\perp$ are the projections of ξ_A and ξ_B, respectively, on the orthogonal complement of χ. In particular,

$$\Delta A(\rho)^2 = (A,A) - AA \geq \frac{\hbar}{2}\{A,A\}_g(\rho). \tag{11}$$

Let $X_{\hat{A}}^{||}$ and $X_{\hat{B}}^{||}$ be the horizontal components of $X_{\hat{A}}$ and $X_{\hat{B}}$. Cauchy-Schwartz inequality yields

$$G\left(X_{\hat{A}}^{||},X_{\hat{A}}^{||}\right)G\left(X_{\hat{B}}^{||},X_{\hat{B}}^{||}\right) \geq G\left(X_{\hat{A}}^{||},X_{\hat{B}}^{||}\right)^2 + \Omega\left(X_{\hat{A}}^{||},X_{\hat{B}}^{||}\right)^2.$$

Equivalently,

$$\{A,A\}_g\{B,B\}_g \geq \{A,B\}_g^2 + \{A,B\}_\omega^2. \tag{12}$$

This estimate together with (11) imply the geometric uncertainty relation:

$$\Delta A\Delta B \geq \frac{\hbar}{2}\sqrt{\{A,B\}_g^2 + \{A,B\}_\omega^2}. \tag{13}$$

The uncertainty relation (13) agrees with the geometric uncertainty relation derived in [3] for systems in pure states. This is not a coincidence since the pure state case correspond to $\sigma = (1)$. (This does not mean that (13) is independent of σ because g and ω are "spectral weighted".) For systems in pure states, (13) is a geometric version of (7). But for general mixed states the two uncertainty relations are not equivalent, which we make explicit in the next paragraph.

B. Comparison of the uncertainty relations

Using the geometric expressions (8) and (9) for the expectation value functions of $\hat{A}$ and $\hat{B}$, and their symmetric and antisymmetric products, we can give a short geometric proof of the Robertson-Schrödinger uncertainty relation (7). Equations (8), (9) and (10) yield

$$\Delta A^2\Delta B^2 = \frac{\hbar^2}{4}\Big(\{A,A\}_g\{B,B\}_g + \{A,A\}_g\xi_B^\perp\cdot\xi_B^\perp + \{B,B\}_g\xi_A^\perp\cdot\xi_A^\perp + \left(\xi_A^\perp\cdot\xi_A^\perp\right)\left(\xi_B^\perp\cdot\xi_B^\perp\right)\Big), \tag{14}$$

$$((A,B)-AB)^2 + [A,B]^2 = \frac{\hbar^2}{4}\Big(\{A,B\}_g^2 + \{A,B\}_\omega^2 + 2\{A,B\}_g\xi_A^\perp\cdot\xi_B^\perp + \left(\xi_A^\perp\cdot\xi_B^\perp\right)^2\Big). \tag{15}$$

Now (7) follows from (12), (14), (15), and

$$\{A,A\}_g\xi_B^\perp\cdot\xi_B^\perp + \{B,B\}_g\xi_A^\perp\cdot\xi_A^\perp \geq 2\{A,B\}_g\xi_A^\perp\cdot\xi_B^\perp,$$
$$\left(\xi_A^\perp\cdot\xi_A^\perp\right)\left(\xi_B^\perp\cdot\xi_B^\perp\right) \geq \left(\xi_A^\perp\cdot\xi_B^\perp\right)^2.$$

If $2\{A,B\}_g\xi_A^\perp\cdot\xi_B^\perp + \left(\xi_A^\perp\cdot\xi_B^\perp\right)^2 = 0$, then, according to (15), the relation (13) is a geometric equivalent of (7). This is, e.g., the case if $\hat{A}$ or $\hat{B}$ is parallel, or if the density operators in $\mathscr{D}(\sigma)$ represent pure states, in which case the vertical bundle has 1-dimensional fibers. In general, however, the two relations are not equivalent. Equation (15) tells us that the right hand side of (13) interpolates between the two sides of (7) if $2\{A,B\}_g\xi_A^\perp\cdot\xi_B^\perp + \left(\xi_A^\perp\cdot\xi_B^\perp\right)^2 < 0$, and that the right hand side of (7) interpolates between the two sides of (13) if $2\{A,B\}_g\xi_A^\perp\cdot\xi_B^\perp + \left(\xi_A^\perp\cdot\xi_B^\perp\right)^2 > 0$.

IV. EXAMPLE: AN ENSEMBLE OF SPINS

Let $\hat{\mathbf{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ be the spin operator, and write $|s,\mu\rangle$ for the state which is certain to have spin s and magnetic quantum number μ. Recall that $|s,\mu\rangle$ is the common eigenstate of $\hat{S}^2$ and $\hat{S}_z$ such that $\hat{S}^2|s,\mu\rangle = \hbar^2 s(s+1)|s,\mu\rangle$ and $S_z|s,\mu\rangle = \hbar\mu|s,\mu\rangle$. Also recall that

$$\hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-), \quad \hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-), \tag{16}$$

where the raising and lowering operators $\hat{S}_+$ and $\hat{S}_-$ are defined by

$$\hat{S}_\pm|s,\mu\rangle = \hbar\sqrt{s(s+1)-\mu(\mu\pm 1)}\,|s,\mu\pm 1\rangle. \tag{17}$$

Consider an ensemble of spin-s particles, so prepared that the proportion of particles having quantum number μ_j is p_j, $j = 1,2,\ldots k$. The spin part of the ensemble's wave function can be represented by the density operator $\rho = \sum_j p_j|s,\mu_j\rangle\langle s,\mu_j|$, and we assume that we are in the generic nondegenerate situation $p_1 > p_2 > \cdots > p_k$.

The map $\psi = \sum_j \sqrt{p_j}|s,\mu_j\rangle e_j^\dagger$ sits in the fiber over ρ, and (6),(16), and (17) yield

$$\begin{aligned} X_{\hat{S}_x}(\psi) &= \frac{1}{2i}\sum_j \big(a_j^+|s,\mu_j+1\rangle + a_j^-|s,\mu_j-1\rangle\big)e_j^\dagger, \\ X_{\hat{S}_y}(\psi) &= -\frac{1}{2}\sum_j \big(a_j^+|s,\mu_j+1\rangle - a_j^-|s,\mu_j-1\rangle\big)e_j^\dagger, \end{aligned}$$

where $a_j^\pm = \sqrt{s(s+1)-\mu_j(\mu_j\pm 1)}$. These vectors are horizontal because the spectrum of ρ is nondegenerate and the matrices $\psi^\dagger X_{\hat{S}_x}(\psi)$ and $\psi^\dagger X_{\hat{S}_y}(\psi)$ have only zeros on their diagonals. (Hence replacing $\psi^\dagger X$ in (5) with $\psi^\dagger X_{\hat{S}_x}(\psi)$ or $\psi^\dagger X_{\hat{S}_y}(\psi)$ will make the right hand side of (5) vanish.) Now,

$$\begin{aligned} \{S_x,S_y\}_g(\rho) &= 2\hbar\Re\operatorname{Tr}\big(X_{\hat{S}_x}(\psi)^\dagger X_{\hat{S}_y}(\psi)\big) = 0, \\ \{S_x,S_y\}_\omega(\rho) &= 2\hbar\Im\operatorname{Tr}\big(X_{\hat{S}_x}(\psi)^\dagger X_{\hat{S}_y}(\psi)\big) = \hbar\sum_j p_j\mu_j. \end{aligned}$$

Consequently,

$$\Delta S_x(\rho)\Delta S_y(\rho) \geq \frac{\hbar^2}{2}\Big|\sum_j p_j\mu_j\Big|. \tag{18}$$

Not surprisingly, one identifies the right hand side of (18) as $\hbar/2$ times the modulus of $S_z(\rho)$.

V. CONCLUSION

In this paper we have equipped the orbits of isospectral density operators, i.e., the phase spaces of unitarily evolving quantum systems in mixed states, with Riemannian and symplectic structures, and we have derived a geometric uncertainty principle for observables acting on quantum systems in mixed states. Also, we have compared this uncertainty relation with the Robertson-Schrödinger uncertainty relation.

The fact that the phase spaces for unitarily evolving quantum systems in mixed states admits Riemannian and symplectic structures g and ω, and, as we will show in a forthcoming paper, an almost complex structure J that makes (ω, J, g) a *compatible triple* [9], opens up for an elegant geometric formulation of quantum mechanics for systems in mixed states. The authors will delve deeper into this issue in a series of forthcoming papers.

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